# Evidence of first-order transition between vortex glass and Bragg glass phases in high-$T_c$ superconductors with point pins: Monte Carlo simulations

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Phase transition between the vortex glass and the Bragg glass phases in high-$T_c$ superconductors in $\vec{B} \parallel \vec{c}$ is studied by Monte Carlo simulations in the presence of point pins. A finite latent heat and a $\delta$-function peak of the specific heat are observed, which clearly indicates that this is a thermodynamic first-order phase transition. Values of the entropy jump and the Lindemann number are consistent with those of melting transitions. A large jump of the inter-layer phase difference is consistent with the recent Josephson plasma resonance experiment of $Bi_2Sr_2CaCu_2O_{8+y}$ by Gaifullin *et al.*

74.60.Ge, 74.62.Dh, 74.25.Dw

Vortex states in high-$T_c$ superconductors have been intensively studied experimentally and theoretically [1]. Because of large fluctuations owing to high transition temperature and strong anisotropy, the flux-line lattice (FLL) melts at much lower temperatures than those predicted by Abrikosov's mean-field theory. The FLL melting is a thermodynamic first-order phase transition. In pure systems, the melting line stretches up to a high magnetic field as large as $H_{c_2}$. However, all experiments show that first-order melting lines terminate at much lower magnetic fields [2,3]. Complicated phase diagrams are obtained experimentally in $Bi_2Sr_2CaCu_2O_{8+y}$ (BSCCO) [4] and $YBa_2Cu_3O_{7-\delta}$ (YBCO) [5], and it is believed that effects of impurities are essential in real materials. For example, vacancies of oxygen atoms, which play the role of point pins to flux lines, cannot be excluded completely even in crystals of highest quality.

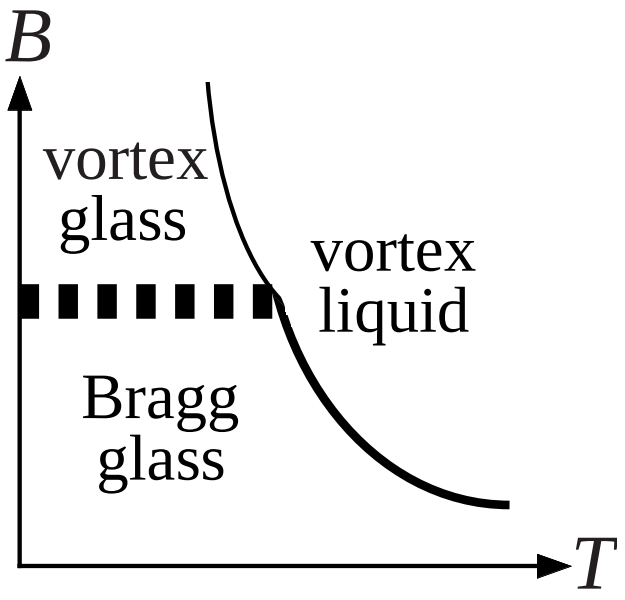


FIG. 1. Schematic vortex phase diagram of high-$T_c$ superconductors with point pins.

Fisher *et al.* [6] studied the Ginzburg-Landau model in a random potential, and proposed the so-called vortex glass (VG) phase before experimental studies. Giamarchi and Doussal [7] pointed out that the Bragg glass (BG) phase can exist in weak fields. In this phase, correlation functions decay in power laws [8,9], and the structure factor shows a triangular Bragg pattern. Accordingly, a phase transition between these two glass phases may be observed when the magnetic field is sweeped across the phase boundary (see Fig. 1). The existence of the VG–BG phase transition in vortex systems with point pins shows a sharp contrast to the phase diagram of pure systems. Presuming a first-order phase transition, the VG–BG phase boundary was evaluated phenomenologically [10,11]. However, physical properties around this phase boundary have not been clarified in experiments and numerical calculations until recently. The shape of the phase boundary seems to depend on observed quantities, and some experiments even suggest a crossover rather than a phase transition. Although some simulations [12–15] gave phase diagrams similar to that of Giamarchi and Doussal, numerical accuracy of these studies was not good enough to distinguish phase transitions and crossovers. The stability of the VG phase was studied by Kawamura [16] including the screening effect.

Quite recently, Gaifullin *et al.* observed [17] a large jump of the inter-layer phase difference on the VG–BG phase boundary of BSCCO by the Josephson plasma resonance experiment. They claimed that their observation is the evidence of a first-order phase transition. In the present Letter, we show more direct evidence of the first-order phase transition on the VG–BG boundary by large-scale Monte Carlo simulations. That is, a finite latent heat and a $\delta$-function peak of the specific heat are observed. Sharp jumps of the inter-layer phase difference and the averaged fluctuations of flux lines are also obtained.

In order to clarify vortex states and phase transitions of high-$T_c$ superconductors in the presence of point pins, we start from the three-dimensional anisotropic, frustrated XY model on a simple cubic lattice [18,19]. Effects of

point pins are introduced into the model by randomly-distributed weakly-coupled plaquettes in the $ab$ plane. Since a vortex sitting on a plaquette costs an energy proportional to the couplings surrounding it, flux lines tend to penetrate plaquettes with weaker couplings in order to reduce such loss of energies. The Hamiltonian of our model is given by

$$H = -\sum_{i,j\in ab \text{ plane}} J_{ij}\cos\left(\phi_i - \phi_j - A_{ij}\right) - \frac{J}{\Gamma^2}\sum_{m,n\|c \text{ axis}} \cos\left(\phi_m - \phi_n\right) \ , \quad (1)$$

$$A_{ij} = \frac{2\pi}{\Phi_0}\int_i^j \mathbf{A}^{(2)}\cdot \mathrm{d}\mathbf{r}^{(2)}, \quad (2)$$

with the periodic boundary condition along all the directions. Couplings in the $ab$ plane are given by $J_{ij} = bJ$ $(0 < b < 1)$ on the weakly-coupled plaquettes, and $J_{ij} = J$ otherwise. The density and the strength of point pins are controlled by the probability of weakly-coupled plaquettes, $p$, and the parameter $b$, respectively (see Fig. 2). The pinning energy is of order of $(1-b)J$. A uniform magnetic field is applied along the $c$ axis, and its strength is proportional to the averaged number of flux lines per plaquette, $f$. Here we concentrate on the model with $L_x = L_y = 50$ and $L_c = 40$. This system size is large enough to describe the melting transition in the pure system $(b = 1)$ [19].

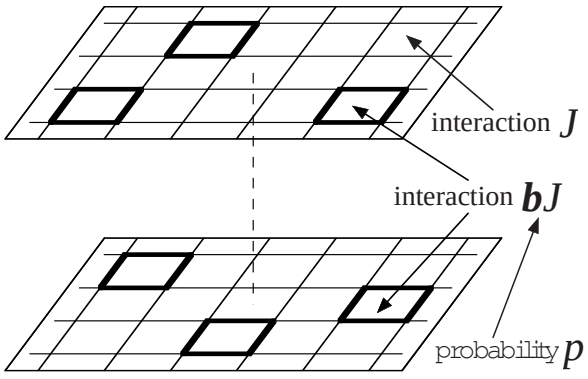


FIG. 2. Schematic description of point pins in the present model.

In our model, we have four adjustable parameters: the anisotropy constant $\Gamma$, the density of flux lines $f$, the density of point pins $p$, and the strength of point pinning $b$. In order to investigate the VG–BG transition, we vary $b$, while fix the temperature at $T = 0.06J/k_{\mathrm{B}}$ and other parameters at $\Gamma = 20$, $f = 1/25$ and $p = 0.003$. In other words, material parameters of the bulk system and the number and positions of point pins are not changed during the simulations. As will be shown later, this temperature is low enough for the study of the VG–BG phase boundary. Typical Monte Carlo steps (MCS) with the Metropolis algorithm are $3 \sim 4 \times 10^7$ MCS for equilibration, and $0.5 \sim 1 \times 10^7$ MCS for measurement.

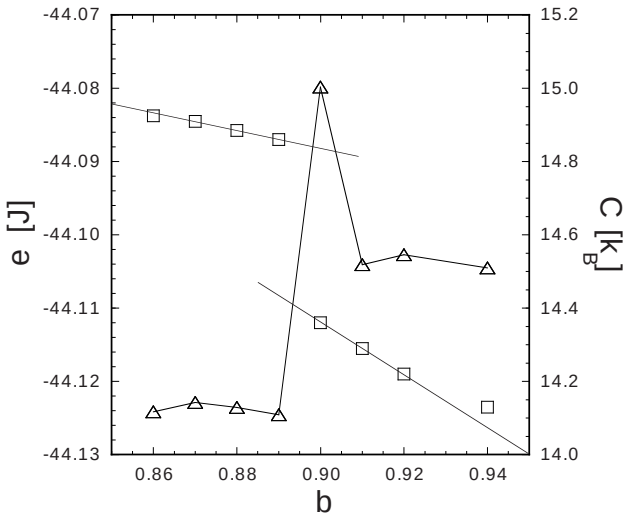


FIG. 3. Internal energy $e$ (squares) and specific heat $C$ (triangles) per flux line per $ab$ plane versus strength of point pinning $b$. Straight lines are drawn as guides for eyes.

First, the $b$ dependence of the internal energy $e$ and the specific heat $C$ per flux line per $ab$ plane is displayed in Fig. 3. Clearly, the internal energy shows a sharp jump at the transition point $b^* = 0.895 \pm 0.005$ with a latent heat per flux line per $ab$ plane $Q \approx 2.3 \times 10^{-2}J$, and a $\delta$-function peak of the specific heat also occurs at the same parameter. These two facts indicate that the VG–BG transition is a thermodynamic first-order phase transition. From this latent heat, the entropy jump at $b^*$ is estimated as

$$\Delta S = Q/T \approx 0.38 k_{\mathrm{B}}, \quad (3)$$

which is comparable to the experimental value in the melting transition of YBCO, $\Delta S \approx 0.5 k_{\mathrm{B}}$ [20].

Second, the $b$ dependence of the inter-layer phase difference, $\langle\cos(\phi_n - \phi_{n+1})\rangle$, is plotted in Fig. 4. This quantity is related to the Josephson energy per phase variable $e_{\mathrm{J}}$ and the anisotropy constant $\Gamma$ as

$$\langle\cos(\phi_n - \phi_{n+1})\rangle = -e_{\mathrm{J}}\Gamma^2/J, \quad (4)$$

and a small change of $e_{\mathrm{J}}$ is magnified in this quantity in extremely anisotropic systems. This quantity also jumps sharply at $b^* = 0.895 \pm 0.005$, and the value of the jump at $b^*$, $\Delta_{\mathrm{PD}} \approx 0.12$, is as large as the experimental value, $\Delta_{\mathrm{PD}} \approx 0.2$ [17]. Moreover, the ratio of the jump of the Josephson energy to the latent heat is given by $\Delta e_{\mathrm{J}}/(Qf) \approx 0.34$, which means that the latent heat is equally distributed to all the directions in the VG–BG phase transition in extremely anisotropic systems.

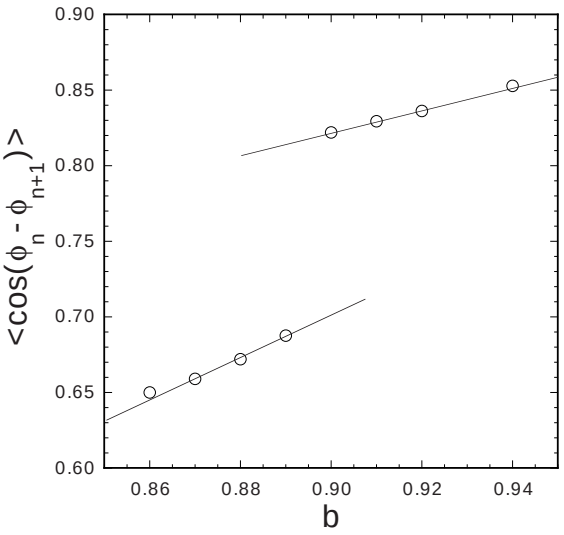


FIG. 4. Inter-layer phase difference $\langle\cos(\phi_n - \phi_{n+1})\rangle$ versus strength of point pinning $b$. Straight lines are drawn as guides for eyes.

Third, the Lindemann number is evaluated directly [21]. The deviation $u$ of a flux line is measured in each $ab$ plane from the projection of the mass center of the flux line, and averaged over all the flux lines and the $ab$ planes. Then, the Lindemann number $c_{\rm L}$ is given by

$$c_{\rm L} = \lim_{b \to b^* + 0} \langle u^2 \rangle^{1/2} / a_0 \ , \tag{5}$$

with the lattice constant of the triangular FLL, $a_0 = (2/\sqrt{3})^{1/2}/f^{1/2}$. The $b$ dependence of $\langle u^2 \rangle^{1/2}/a_0$ is shown in Fig. 5, and we have $c_{\rm L} \approx 0.28$. This value is almost equal to the one obtained in the FLL melting of pure systems [21].

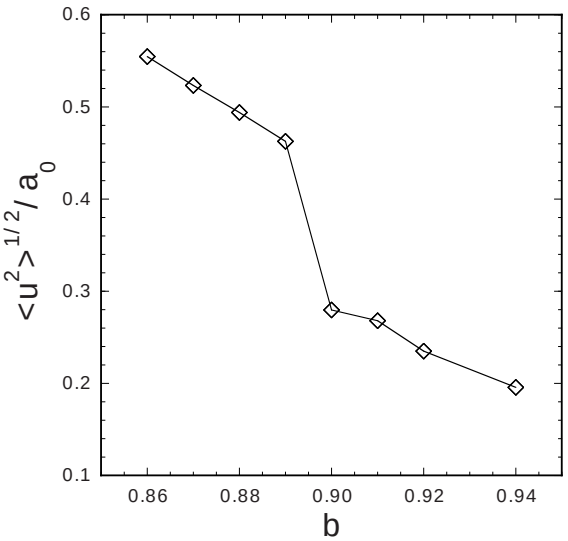


FIG. 5. Averaged fluctuations of flux lines $\langle u^2 \rangle^{1/2}/a_0$ versus strength of point pinning $b$.

Finally, we go into some details of the present simulations. The system with $b = 0.90$ is calculated at first. Simulations are started from a random configuration at a very high temperature, and the system is gradually cooled down to $T = 0.06 J/k_{\rm B}$. During the cooling process, the first-order melting transition characterized by a discontinuous appearance of the helicity modulus along the $c$ axis, $\Upsilon_c$ [19], takes place at $T_{\rm m} \approx 0.079 J/k_{\rm B}$, which corresponds to the vortex liquid (VL)–BG phase transition. Then, the strength of point pinning $b$ is varied. Since the quantity $\Upsilon_c$ is proportional to the superfluid density, the region with finite $\Upsilon_c$ is superconducting. This quantity is nonvanishing for all the values of $b$ shown in Figs. 3–5 at $T = 0.06 J/k_{\rm B}$, and therefore the phase transition investigated in the present Letter is not the VL–BG one, but the VG–BG one. Equilibration in systems with point pins is much slower than that in pure systems, and only one sample can be taken for calculations at present. Nevertheless, the results obtained in the present Letter are quite clear-cut and consistent with experiments. Thus, the small number of random sampling does not seem serious. Since positions of point pins are independent in each $ab$ plane, the number of $ab$ planes, $L_c = 40$, would be large enough for averaging effects of point pins.

Although we have concentrated on the VG–BG transition for a single density of point pins $p$ in the present Letter, we have also investigated the VL–BG and VL–VG transitions for various $p$, and obtained the overall phase diagram in the $p$–$T$ plane. The structure of the $p$–$T$ phase diagram is similar to that of the $B$–$T$ phase diagram. Experimentally, the increase of $p$ corresponds to the repeated irradiation of electrons or protons, and our $p$–$T$ phase diagram is consistent with recent experiments [22,23]. Details of this study will be reported elsewhere [24].

In conclusion, the first thermodynamic evidence of the first-order transition between the vortex glass (VG) and the Bragg glass (BG) phases has been obtained in high-$T_{\rm c}$ superconductors in the presence of point pins. A finite latent heat and a $\delta$-function peak of the specific heat are observed by large-scale Monte Carlo simulations of the three-dimensional anisotropic, frustrated XY model with randomly-distributed weakly-coupled plaquettes. The entropy jump derived from the latent heat is nearly equal to those in the melting transition of YBCO. The Lindemann number evaluated from fluctuations of flux lines, $c_{\rm L} \approx 0.28$, is reasonable for the first-order phase transition. The inter-layer phase difference also shows a sharp jump on the VG–BG phase boundary. This property is consistent with the Josephson plasma resonance experiment of BSCCO by Gaifullin *et al.*

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